201-16018B

IUCLID

Data Set

Existing Chemical	:	ID: 88230-35-7
CAS No.	:	88230-35-7
TSCA Name	:	Hexanol, acetate, branched and linear
Molecular Formula	:	Unspecified
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Status	:	
Memo	:	ExxonMobil HPV
Printing date	:	19.04.2005
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Number of pages	:	31
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the alkyl acetates category.

Remark : Alkyl Acetates follow a regular pattern as a result of synthesis and structural similarity. Aliphatic, monohydric alcohols are reacted with acetic acid to form the corresponding acetate esters (CH3COOR).
Members associated with this template category are:
88230-35-7 Hexanol, acetate, branched and linear
90438-79-2 Acetic acid, C6-8 branched alkyl esters
108419-32-5 Acetic acid, C7-9 branched alkyl esters
108419-33-6 Acetic acid, C8-10 branched alkyl esters
108419-34-7 Acetic acid, C9-11 branched alkyl esters
108419-35-8 Acetic acid, C11-14 branched alkyl esters

07.12.2000

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

C6 branched and linear alkyl acetate ester

07.12.2000

Exxate 600

09.02.2001

Oxo-hexyl acetate

27.05.2004

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -59 °C
Sublimation	:	
Method	:	other: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: Hexyl acetate ester
Method	:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Remark	:	EPIWIN is used and advocated by the USEPA for chemical property estimation.
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (2)

2.2 BOILING POINT

Value	:	= 164 - 176 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078 Mod
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

04.06.2004 (15)

2.3 DENSITY

Type	:	relative density
Value	:	= .87 at 20 °C
Method	:	other: ASTM D891
Year	:	
GLP	:	no data
Test substance	:	other TS

Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint
04.06.2004		(15)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 1.93 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	
GLP	:	no data
Test substance	:	other TS: hexyl acetate ester
Test condition	:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
19.04.2005		(2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 2.83 at 25 °C
pH value	:	
Method	:	other (calculated): Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year	:	
GLP	:	no data
Test substance	:	other TS: hexyl acetate ester
Test condition	:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data

are calculated and not measured.

Flag : Critical study for SIDS endpoint
19.04.2005 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 309 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year	:	
GLP	:	no data
Test substance	:	other TS: hexyl acetate ester
Test condition	:	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	no
Test substance	:	other TS: hexyl acetate ester
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Acetates C6 to C13 category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis. These data indicate that photolysis will not significantly contribute to the degradation of alkyl acetate esters in the aquatic environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York,

USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : Hexyl acetate ester
Flag : Critical study for SIDS endpoint
19.04.2005

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .0000000000074355 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no data
Test substance : other TS: hexyl acetate ester

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
17.3	7.43 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on

the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : Hexyl acetate ester
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
19.04.2005 (2)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : = 13 day(s) at 25 °C
t1/2 pH 9 : = 36 day(s) at 15 °C
Deg. product : not measured
Method : OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year : 1992
GLP : yes
Test substance : other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)

Result : Half life at pH 9 and 25 Deg C = 13 days.
Half life at pH 9 and 15 Deg C = 36 days.

The test substance was hydrolytically stable at pH 4, and pH 7 as it degraded less than 5% in 5 days.

Test substance hydrolysis was observed at pH 9 with 35% degradation observed after Day 1 and 95% at Day 5. Test substance measured analytically by GC-FID.

Test condition : The hydrolysis of the test substance was evaluated at 3 relevant pH values. A preliminary test of 95ug/ml at pH values of 4, 7, and 9, showed stability at pH 4 and pH 7. A definitive test was performed at 98ug/ml and a pH value of 9 at varying temperatures (15 and 25 Deg C).
Sufficient volumes of test substance stock solution were added to buffer solution to yield a nominal concentration of 98ug/ml (less than half of expected water sol. conc.). Samples were stored in the dark in laboratory incubators and the temperature recorded daily.

Test vessels were sterilized VOA vials containing buffer solutions of the test substance, with no headspace.

Test substance : CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Conclusion : Hydrolysis of the test substance is not expected to be a significant mechanism of abiotic degradation in natural bodies of water where the temperature is generally less than 25 Deg C and the pH is at or below 7.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (6)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	1998
Method	:	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). Input values used: Molecular mass = 144.22 g/mol Water solubility = 309 mg/L Vapour pressure = 193 Pa log Kow = 2.83 Melting point = -59 deg C
Result	:	Air- 91.9% Water- 5.0% Soil- 3.0% Sediment - <0.1% Suspended Sed - <0.01% Biota - <0.01%
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (19)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: Domestic activated sludge, raw sewage, and soil
Contact time	:	28 day(s)
Degradation	:	= 76.9 (±) % after 28 day(s)
Result	:	readily biodegradable
Deg. product	:	

Method	:	EPA OTS 796.3100
Year	:	1988
GLP	:	yes
Test substance	:	other TS: CAS No. 110-82-7; C6 methyl-branched and linear alkyl acetate ester

Result : Half-life was <=2 weeks. By day 28, 76.9% degradation of the test material was observed. 10% biodegradation was achieved on approximately day 2, 50% biodegradation on approximately day 13.
By day 7, >60% biodegradation of positive control was observed. No excursions from the protocol were noted.
Biodegradation was based on theoretical Carbon Dioxide values and the cumulative Carbon Dioxide produced by the test substances.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Substance	74.6, 82.0, 74.1	76.9
Aniline	86.5, 83.7, 83.9	84.7

* replicate data

Test Substance
% Degradation
(mean of replicate data)
Day 2 = 9.7
Day 5 = 30.7
Day 13 = 55.8
Day 19 = 68.2
Day 28 = 76.9

Test condition : Although this test procedure uses an acclimated inoculum, the study was conducted with a non acclimated inoculum that contained activated sludge, raw sewage, and soil. The inoculum and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 2L Gledhill flasks located in the dark in an environmental chamber. Each test vessel was monitored for carbon dioxide via charcoal tube and air purging. Sampling was performed on Days 2, 3, 5, 7, 13, 19, and 28.
Test material and positive control were tested in triplicate.
Test material concentration was 30mg carbon/L. Aniline (positive control) concentration was 20 mg carbon/L.
Test temperature was 19 to 23 Deg C.

Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

19.04.2005 (3)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	other: see remark
Exposure period	:	at °C
Concentration	:	
BCF	:	= 30
Elimination	:	
Method	:	other: calculation
Year	:	
GLP	:	no data
Test substance	:	other TS: hexyl acetate ester

Remark	:	A log BCF of 1.5 (BCF = 30) is calculated. Hexyl acetate ester in the aquatic environment is expected to have a low potential for bioaccumulation. The SMILES notation used was CC(=O)OCCCCCC
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag 19.04.2005	:	Critical study for SIDS endpoint

(1)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LL50	:	= 11.9 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1992
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Result	:	96 hour LL50 = 11.9 mg/L (95% CI 10.6 to 13.4) based upon nominal values. The fish were slightly smaller than the guideline suggestion of 4.0 to 6.0cm, which were purposely selected to help maintain oxygen levels in the closed system.

Nominal Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
0.5	0
1.3	0
3.2	0
8.0	1
20.0	15

*15 fish added at test initiation
Statistical Method: Trimmed Spearman Karber Method

Test condition	:	The analytical method measured Total Organic Carbon (TOC). TOC was monitored throughout the study in new and old exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TOC for each level tested. No significantly high or low levels were seen. Individual exposure solutions were prepared by adding the test substance to 17L of laboratory blend water in 20L glass carboys. The solutions were mixed for 24 hours at test temp (13-17 Deg C) with a vortex of <10%. Mixing was performed using a magnetic stir plate and teflon stir bar (132 rpm). After mixing, the solutions were allowed to settle for one hour and the Water Accommodated Fraction (WAF) was removed via a glass tube from the bottom of vessel. Test vessels were 4.0L aspirator bottles containing 4.5L of solution (no headspace). Test vessels were sealed with foil covered stoppers. Three replicates of each concentration were tested, each containing 5 fish. Approximately 80% of each solution was renewed daily from a freshly prepared WAF. Nominal treatment levels were control, 0.5, 1.3, 3.2, 8.0, and 20.0mg/L Test temperature was 15.2 Deg C. Lighting was 62 to 69 ft. candles with gradual 16 hrs light and 8 hrs dark. Dissolved oxygen was 9.0 to 9.4mg/L for "new" solutions and 6.3 to 8.5mg/L for "old" solutions. The pH ranged from 7.4 to 7.7 for "new" solutions and 7.0 to 7.4 for "old" solutions. Fish supplied by Thomas Fish Co.; age = approximately 6 weeks; mean wt.=0.333g; mean total length=3.6cm; test loading=0.37g of fish/L.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
LL50	:	= 7.6 measured/nominal
Limit Test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	1992
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)

Result : 48 hour LL50 = 7.6 mg/L (95% CI 5.9 to 10.7mg/L) based upon nominal values.

Analytical method used was Total Organic Carbon (TOC).

Nominal Conc. (mg/L)	Daphnia Total Mortality (@48 hrs)*
Control	1
0.1	2
0.5	1
1.0	3
5.0	5
10.0	14

*20 Daphids total added at test initiation.
Mortality is defined as immobilized.
Statistical Method: Finney, D.J. probit procedure of SAS

The analytical method measured Total Organic Carbon (TOC). TOC was monitored throughout the study in new and old exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TOC for each level tested. No significantly high or low levels were seen.

Test condition : Individual exposure solutions were prepared as water accommodated fractions (WAFs). A WAF was prepared by adding test substance to 1.8L of solution in a 2.0 liter aspirator bottle and mixing with a magnetic stir plate and bar. Mixing vortex was <10%. After mixing for 24 hours at room temperature, the WAF was allowed to settle for one hour and removed from the port at the bottom of the bottle.
Test vessels were 125ml glass beakers filled with 140ml of solution and covered. Four replicates were prepared for each treatment. Each replicate contained 5 organisms.
Nominal treatment levels were: control, 0.1, 0.5, 1.0, 5.0, and 10.0mg/L
Test temperature was 20.7 Deg C. Lighting was 58 to 59 ft candles with 16 hrs light and 8 hrs dark. Dissolved oxygen was 7.3 to 8.8mg/L. The pH ranged from 7.3 to 8.3.

Organisms were supplied by in-house cultures; age = <24 hours old. Parents age = 14 to 18 days old.

Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (7)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	growth rate
Exposure period	:	96 hour(s)
Unit	:	mg/l
EL50 (biomass)	:	= 40.1 measured/nominal
EL50 (growth rate)	:	= 32.1 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	1992
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)

Result :

96 hour EL50b = 40.1 mg/L (biomass) based upon nominal values
96 hour EL50gr = 32.1 mg/L (growth rate) based upon nominal values
NOELRb = 31.0 mg/L (biomass) based upon nominal values
NOELRgr = 8.0 mg/L (growth rate) based upon nominal values

No excursions from the protocol were noted.

Nominal Conc. (mg/L)	Mean Growth - 72 & 96 hr (% Inhibition)		Cell Conc. - 96 hr (cells/ml)
Control	n/a	n/a	8.8 x10(5)
8.0	1.2	-4.2*	1.1 x10(6)
31.0	8.4	-3.5*	1.1 x10(6)
62.0	80.2	84.4	2.6 x10(4)
125.0	94.5	97.2	9.6 x10(3)
250.0	99.9	100.0	3.4 x10(3)

n/a - Not applicable
*Stimulatory response
Statistical Method: Proc regression procedure of SAS, Anova procedure of SAS for NOEC

The analytical method measured Dissolved Organic Carbon (DOC). DOC was monitored throughout the study in new and old exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of DOC for each level tested. No significantly high or low levels were seen.

Test condition : Individual exposure solutions were prepared as Water Accommodated Fractions (WAFs). Test material was added to 1.8L of algal media in 2.0L aspirator bottles. The mixing vessels were sealed with foil covered stoppers and mixed on magnetic stir plates with teflon coated stir bars for 24 hours at room temperature. After mixing the solutions were allowed to settle for one hour and the WAF was removed from the bottom of the mixing vessel via the port and used for testing. Test vessels were 125ml glass Erlenmeyer flasks that were completely filled (140ml) with treatment solution and inoculated with algae. Samples were taken daily for cell counts. Four replicates were prepared for each treatment level. The initial algal concentration was 1.0 x 104 cells/ml. All test replicates were placed on a shaker table at 100 oscillations per minute during the study. To facilitate mixing, with no headspace, 10 glass beads were placed in each vessel. Biomass was calculated as the area under the growth curve. Nominal treatment levels were 8.0, 31.0, 62, 125, and 250mg/L

Test temperature was 23.6 Deg. C. Lighting was continuous at 4300 to 4663 Lux. The pH was 7.5 at test initiation and ranged from 8.3 to 10.4 at

test termination.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (5)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 10000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	5
Vehicle	:	other: Corn oil (1.0 % or 10 % v/v)
Doses	:	
Method	:	other: Experimental (Non-regulatory)
Year	:	1963
GLP	:	no
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Oral Gavage. Number of animals per dose = 5. Doses: 34.6, 120, 417, 1450, 5000, or 10,000 mg/kg. Single dose following 3-4 hour-fast. Post dose observation period: 1, 4, and 24 hours postdosing and daily for 14 days. One animal at the 1450 mg/kg dose level died on day 11. No toxic signs were observed prior to death and a normal body weight-gain was recorded at death. Postmortem examination showed congestion of the lungs, kidneys, adrenals, and pancreas, and gaseous distention of the stomach and large intestine at the time of death. All other animals showed no gross pathology following termination. Principal toxic effects seen only at the 10,000 mg/kg dose were depression, ataxia, sprawling of limbs and depressed righting reflex only at the 24-hour observation.
Conclusion	:	The acute oral LD50 for C6 branched and linear alkyl acetate ester in male Sprague-Dawley rats is >10 g/kg.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.

19.04.2005 (16)

Type	:	other: Limit
Value	:	> 2000 mg/kg bw
Species	:	rat
Strain	:	other: Crl:CDBR
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: none
Doses	:	2000 mg/kg
Method	:	other: Experimental (EU Annex V, B.1 and OECD 401)
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Oral Gavage. Number of animals per dose per sex = 5. Single Dose of 2000 mg/kg. Post dose observation period 14 days. There was one female death on Day 0 at the 2-hour observation considered to be the result of test material aspiration during dosing.

Clinical signs of toxicity were limited to nasal, oral and/or ocular discharge, abdominal and/or anogenital staining, and/or soft stool in four males at the Day 0 interval. One male and 4 females were free of abnormalities during the entire study. No gross abnormalities were seen at postmortem examination.

Conclusion : C6 branched and linear alkyl acetate ester, did not elicit signs of acute systemic toxicity when administered orally. Signs of slight toxicity (staining of the fur and soft stool) were limited to the male animals on Day 0. There was one female death on Day 0, but the death was the result of test material aspiration, not toxicity.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint

19.04.2005 (10)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type : other: Limit
Value : > 3160 mg/kg bw
Species : rabbit
Strain : other: albino
Sex : male/female
Number of animals : 1
Vehicle : other: none
Doses :
Method : other: Experimental (Non-regulatory)
Year : 1963
GLP : no
Test substance : other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)

Remark : Dermal Application. Number of animals per dose per sex = 1. Doses: 50, 200, 794 or 3160 mg/kg. Single application / 24-hour occlusive patch. Post dose observation period 14 days.

Two animals, 200 and 3160 mg/kg dosage levels, showed soft feces or diarrhea for two to four days. One animal, 794 mg/kg dosage level, showed diarrhea during the second week and weight loss at termination. All other animals were normal and showed body weight gains. There were no gross pathological findings at the study termination.

Conclusion : C6 branched and linear alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

19.04.2005 (18)

Type : other: Limit
Value : > 2000 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 5
Vehicle : other: none
Doses : 2000 mg/kg

Method	:	other: Experimental (EU Annex V, B.3; OECD 402)
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Route of administration - Dermal. Number of animals per dose per sex = 5. Single application / 24-hour occlusive patch with 2000 mg/kg. Post dose observation period 14 days. There were no signs of systemic toxicity. Slight dermal irritation was noted in all animals, with the most severe response being observed at the Day 1 observation interval. At post mortem examination, all animals had desquamation at the dose site. In general, dermal responses were considered minimal and transient in nature.
Conclusion	:	C6 branched and linear alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (9)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	100 %
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	6
Vehicle	:	other: none
PDII	:	3.08
Result	:	moderately irritating
Classification	:	
Method	:	other: EU Annex V, B.4; OECD 404
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Primary dermal irritation with male New Zealand White rabbits. Number oa animals per dose = 6. Dermal application - single application / 4-hour semi-occlusive patch of 0.5 ml. Post dose observation period 1, 24, 48, and 72 hours and Day 7. Vehicle: none. All animals survived to study termination, were free of clinical signs, and displayed an increase in body weight during the test period. All animals showed erythema and edema in the first 72 hours. The mean scores were 1.72 (erythema) and 1.17 (edema). All animals were free of erythema and edema at the day 7 observation and the study was terminated.
Conclusion	:	C6 branched and linear alkyl acetate ester is a moderate dermal irritant to rabbit skin.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (14)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	100 %
Dose	:	.1 ml
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	
Result	:	slightly irritating
Classification	:	
Method	:	other: Experimental (Non-regulatory)
Year	:	1963
GLP	:	no
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Draize Ocular Irritation with albino rabbits. Single application of neat material of 0.1 ml into the conjunctival sac of the left eye using the untreated right eye as a control. Post dose observation period 1, 4, and 24 hours postdosing and at 2, 3, 4 and 7 days. Vehicle: none. Ocular irritation was most prominent at the 1-hour observation when the total Draize scores ranged from 8 to 12 (Maximum possible score = 110). Irritation was confined to the conjunctivae and generally consisted of moderate redness, chemosis and discharge. The signs of eye irritation completely subsided in all animals by day 7. Fluorescein examination on day 7 confirmed the absence of any corneal damage.
Result	:	Minimal irritation.
Conclusion	:	C6 branched and linear alkyl acetate ester was a mild reversible irritant (Draize Score = 12) causing minimal irritation.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.

19.04.2005 (17)

Species	:	rabbit
Concentration	:	100 %
Dose	:	.1 ml
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	none
Result	:	slightly irritating
Classification	:	
Method	:	other: EU Annex V, B.5; OECD 405
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Draize Ocular Irritation with male New Zealand White rabbits. Single instillation of neat material of 0.1 ml into the conjunctival sac of the right eye using the untreated left eye as a control. Post dose observation period 1, 24, and 48 hours postdosing. Vehicle: none. Ocular irritation was most prominent at the 1-hour observation when the total Draize scores ranged from 10 to 12 (Maximum possible score = 110).

Irritation was confined to the conjunctivae and generally consisted of redness, chemosis and discharge. The signs of eye irritation completely subsided in all animals by the 72-hour evaluation. Fluorescein examination at 72 hours confirmed the absence of any corneal damage.

Result	:	Minimal Irritation.
Conclusion	:	C6 branched and linear alkyl acetate ester was a mild reversible irritant (Draize Score = 12).
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (13)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	other: Crl:CD BR
Route of admin.	:	gavage
Exposure period	:	28 day
Frequency of treatm.	:	once/day
Post exposure period	:	
Doses	:	0, 100, 500, and 1000 mg/kg/day
Control group	:	yes
NOAEL	:	= 1000 - mg/kg
Method	:	other: EU Annex V, B.7; OECD 407
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	28-Day repeated dose oral toxicity. Doses: 0, 100, 500, and 1000 mg/kg/day. Volume: 5 ml/kg. Vehicle: Corn oil.
Conclusion	:	Oral administration of C6 branched and linear alkyl acetate ester daily to rats for 28 days did not produce any signs of overt systemic toxicity at any dose level tested. There were no treatment-related clinical in-life, gross postmortem or microscopic findings (including adrenal glands, heart, kidneys, liver, lung, spleen, testes and ovaries); no treatment-related mortality; and no adverse effects on body weight, food consumption, clinical laboratory parameters, or organ weights.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (8)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	other: Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of testing	:	Bacterial
Test concentration	:	250, 500, 1000, 2000, and 3000 µg/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with

Result	:	negative
Method	:	other: EU Annex V, B.14; OECD 471
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Species/Strain - S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538. Species/cell type - Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9). Vehicle: DMSO. C6 branched and linear alkyl acetate ester, did not induce significant increases in revertant colonies (> 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains. Toxicity was observed in both the initial and repeat assays in the following strains and dose levels: TA98 at 2000 µg/plate without metabolic activation, and at 3000 µg/plate with and without metabolic activation; TA100 at 2000 and 3000 µg/plate with and without metabolic activation; TA1535 at 2000 µg/plate without metabolic activation; TA1537 at 250, 500, 1000, 2000, and 3000 µg/plate without metabolic activation; and TA1538 at 1000 and 2000 µg/plate without metabolic activation, and at 3000 µg/plate with and without metabolic activation. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.
Test condition	:	There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 250, 500, 1000, 2000, and 3000 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 ºC for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.
Conclusion	:	C6 branched and linear alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested, but was toxic in all strains tested under the conditions of this study.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint
19.04.2005		(12)

Type	:	other: In Vitro Chromosomal Aberration Assay in CHO Cells
System of testing	:	Cultured Chinese hamster ovary (CHO) cells
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	
Result	:	

Method	:	other: Galloway, et al, Development of a standard protocol for in vitro cytogenetic testing with Chinese hamster ovary cells: comparison of results for 22 compounds in two laboratories. Environ. Mutagen. 7:1-51, 1985.
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	C6 branched and linear alkyl acetate ester, reduced cell survival by at least 50% when compared to the vehicle control in the repeat assay: 20-hour harvest without activation and 44-hour harvest with and without metabolic activation. All negative and positive controls used in this study performed in an appropriate manner.
Result	:	C6 branched and linear alkyl acetate ester, was tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. A repeat assay was also performed using 20-hour and 44-hour harvests. For the initial 20-hour harvest data, there was no evidence of a positive dose response nor of any treated group being different from the control in these analyses. For the repeat harvest, the high dose group (550 mg/mL) was statistically different from the vehicle control ($p<0.05$). However, this statistically significant finding (6.5% aberrant cells) was not reproducible. No increase was observed at the 44-hour harvest time. In addition, no increase was observed in the initial assay with metabolic activation at similar dose levels. There was no statistically significant finding in the 44-hour harvest.
Test condition	:	Treatment group doses (14 total in initial and repeat assays) ranged from 250-480 mg/mL in the 20-hour initial test; 230-550 mg/mL in the 20- and 44-hour repeat assays. S9 activation was used in doses ranging from 350-480 mg/mL in the 20-hour initial assay and ranging from 380-550 mg/mL in the 20- and 44-hour repeat assays. Vehicle in all assays was DMSO (not exceeding 1.0% final volume to ensure normal cell viability and growth rate). Positive controls, N-methyl-N-Nitro-N-Nitrosoguanidine (MNNG - clastogen that does not require metabolic activation) and 7,12-Dimethylbenz[a]anthracene (DMBA- clastogen that requires metabolic activation) were used as positive controls in the nonactivated series and activated series, respectively.
Conclusion	:	C6 branched and linear alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 550 mg/mL with and 430 mg/mL without metabolic activation.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag 19.04.2005	:	Critical study for SIDS endpoint

(11)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

Memo : EU RIsk assessent final draft

08.06.2001